

A \underline{k} -space transport analysis of the BEEM spectroscopy of Au/Si Schottky barriers

U. Hohenester, P. Kocevar

Inst. f. Theoretische Physik, Karl-Franzens-Universität Graz, A-8010 Graz (AUSTRIA)

P.L. de Andres and F. Flores

Instituto de Ciencia de Materiales (CSIC), Cantoblanco, E-28049 Madrid (SPAIN)

*Dept. de Fisica Teorica de la Materia Condensada (UAM), Universidad Autonoma de Madrid,
E-28049 Madrid (SPAIN)*

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Abstract

We address the question of the spatial resolution of ballistic electron emission microscopy (BEEM) of Schottky barriers in Au(111)/Si(100) and Au(111)/Si(111) interfaces. A novel combination of Green-function and \underline{k} -space Ensemble-Monte-Carlo techniques is used to obtain new insights into the spatial and energetic evolution of the STM-tip-induced electrons during their passage through the metallic layer before reaching the metal-semiconductor interface. In particular, it is shown how the effect of band-structure-induced directional focusing of the electrons enforces a reinterpretation of existing experimental data.

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I. INTRODUCTION

The recent theoretical prediction (de Andres et al. 1997) of decisive band-structure effects in the propagation of the STM-tip-induced hot electrons through the metal layer brought a new facet to the discussion about the very high spatial resolution of ballistic electron emission microscopy (BEEM) of Au/Si Schottky barriers (Bell 1996; Prietsch 1995). While most interpretations of BEEM data on Au/Si(100) and Au/Si(111) interfaces have assumed a narrow forward cone of tunneling-injected electrons and explained the very similar spectra and their high spatial resolution through various forms of collisional beam broadening, the prediction of a pronounced off-axis shift and broadening of the angular distribution just below the surface reopens the discussion about the role of the band structure and of scattering processes in the bulk and at the boundaries of the metallic layer. It is the purpose of the present analysis to improve the conventional energy-space descriptions and Monte-Carlo

simulations of the hot-electron dynamics by providing a detailed \underline{k} -space Ensemble-Monte-Carlo simulation of the passage of the hot electron through the Au layer, including the essentials of the band structure in the directional spectrum of the injected electrons, in the free-particle propagation, and also in the scattering cross sections for electron-electron (e-e), electron-phonon (e-ph), and electron-boundary scattering. The recent experimental data of Bell (1996) for varying layer thickness d and temperature will be reanalysed and the results contrasted with Bell's original interpretation. It will be shown that the two most intensively debated questions about BEEM spectroscopies of the Au/Si system, namely the questions about the origin of the great similarity between Au/Si(100) and Au/Si(111) spectra and about the extreme high spatial resolution, can, for the first time, be directly answered without the use of adjustable parameters or ad hoc assumptions.

II. TRANSPORT MODEL

Before presenting our transport model, we briefly summarise the conventional model, which is mainly based on the ideas of Kaiser and Bell (1988). The original KB model assumes (i) that the injected distribution at the metal surface is concentrated within a narrow forward cone, (ii) that the \underline{k} -distribution at the metal/semiconductor interface is identical to the injected \underline{k} -distribution at the metal surface, i.e. the \underline{k} -vector parallel to the plane $\underline{k}^{\parallel} \approx 0$, and (iii) that $\underline{k}^{\parallel}$ is conserved at the interface (i.e. specular reflection/transmission via continuity of wavefunctions). As a consequence of the different orientations of the six conduction-band valleys in Si with respect to the impinging narrow forward cone at the interface, BEEM spectra for Au/Si(100) and Au/Si(111) should, in the absence of strong scattering effects, be distinctly different. This should occur because of matching of $\underline{k}^{\parallel}$ for Au/Si(111), a prediction in strong contrast with the experimental facts.

We now turn to our present transport model. We first note that STM and LEED studies show that Au films grow on Si(100) and Si(111) by forming crystals oriented preferentially in the [111] direction. Then the empirical-tight-binding Green function analysis (Garcia-Vidal et al. 1996) of the coherent electron propagation from the STM tip through the tunneling gap into the metal layer reveals that the STM electrons achieve their bulk Bloch character, with propagation gaps due to forbidden regions of phase space, after passing roughly 20 Å within the metal. The injected distribution at $z = 20$ Å turns out to reach its maximum at the edge of the planar Brillouin zone at ≈ 30 degrees (from the normal direction), with an average $1/\cos\theta$ distribution law (de Andres et al. 1977). We should stress that the detailed shape of this distribution depends on the exact tip-surface configuration. **This angular distribution is essentially different from the conventionally assumed narrow forward cone and should drastically change most of the previous interpretations of BEEM data on Au/Si.** The energetic spectrum of the injected electrons is taken from conventional planar tunneling theory (Prietsch 1995).

In view of the fact that the total mean free path is much greater than 20 Å, our Monte-Carlo simulations of the electronic scattering dynamics use the above Green function result as the input ensemble of injected STM electrons at the surface. Appropriately modifying well-established Ensemble-Monte-Carlo techniques for the solution of the non-linear steady-state Boltzmann equation for semiconductors (Hohenester et al. 1992), the hot-electron distribution function $f_{IF}(\underline{k})$ at the interface is obtained as follows. Starting from quasifree

electrons ($m_{eff} = m_0$), we correct for band-structure effects on the electron propagation by cutting off the forbidden directions arising from gaps in the constant-energy surfaces. For our case of injection energies about 1 eV above the Fermi energy, these "propagation gaps" form cones with an opening angle of 10 degrees around the [111] directions and are easily included in the scattering dynamics by use of Monte-Carlo rejection techniques.

The total and differential cross sections for the scattering between the hot electrons and those of the "cold" metallic background are treated via a dynamically screened Coulomb potential (Pines 1968), via the standard Monte-Carlo procedure (Jacoboni and Reggiani 1983). This full \mathbf{k} -space description should be contrasted with the earlier MC simulations of the bulk scattering dynamics in the metal (Bauer et al. 1993, Bell 1996), which are based on an energy-space description, with mean free paths numerically adjusted to the experimental data by use of simple rational functions of energy.

Assuming specular transmission/reflection (via wavefunction matching at a step-like barrier Θ_B) and either specular or diffuse reflection at the free metal surface (both types of reflections resulting in practically identical simulated BEEM currents), the boundary scatterings are treated in the conventional way (Bauer et al. 1993, Bell 1996).

The simulation of each electron is also followed in \mathbf{r} -space and stopped after it has passed the interface (i.e. when $z > d$) or when its energy has dropped below the top of the barrier. In this way one obtains the energetic and angular distribution of transmitted electrons at the interface. We further assume negligible current modifications within the semiconductor, which should be well justified for the modest electron energies of our present concern (Prietsch 1995). Then the relative portion of transmitted electrons directly determines the relative BEEM current I_B/I_T as function of the tunnel bias V_T for the given barrier Θ_B . Four our calculations of the I_B characteristics and analysis of the spatial resolution we used the standard value $\Theta_B = 0.8$ eV; we checked that the known small temperature variation of Θ_B does not change the essentials of our results.

III. RESULTS AND CONCLUSIONS

Although we have analysed both Si orientations, we concentrate our following discussion mainly on Au(111)/Si(111). We first state that, as had already been demonstrated by GF calculations of Garcia-Vidal et al. (1996) and de Andres et al. (1997) for a pure ballistic electron propagation through the metal layer, the comparable I_B thresholds and magnitudes for Au/Si(111) and Au/Si(100) and the high spatial BEEM resolution are a direct consequence of the band structure-induced non-forward electron injection. This claim can now be substantiated by the results of our inclusion of the scattering dynamics in the former free-electron scenario of de Andres et al. (1997). To demonstrate clearly the effect of scattering processes, we first consider the very narrow off-axis initial distribution originally obtained by Garcia-Vidal et al. (1996) within the present GF approach by neglect of self-interference effects in the coherent free-electron propagation. Figure 1 shows the resulting lateral current distribution within the layer (taken as semi-infinite) at three typical penetration depths (left) and its much smaller fraction due to scattered electrons (right; note change of scale). One can easily distinguish the build up of secondary "hot" electrons at the lowest energies due to inelastic e-e scatterings and the angular spreading of the distribution through the quasi-elastic e-ph interactions. For this illustrative example a high spatial

resolution in I_B would be found, caused by the dominance of those "happy" \underline{k} -matching electrons (distributed typically between 35 and 45 degrees within the high-angle wing of the distribution) which cross the interface at their first attempt.

Turning to the initial distribution underlying this study (de Andres et al. 1997), our simulations also yield a high spatial resolution, which again is caused by the fraction of "happy" electrons in the angular range between 35 and 45 degrees, which now lies in the low-angle wing of the distribution. Figure 2 compares our results for the BEEM current characteristics (full lines) with Bell's experimental data (diamonds) for two different layer thicknesses and temperatures. The theoretical curves are in quantitative agreement with the data, except for the case of "thick" layers ($d = 300 \text{ \AA}$) and "low" temperatures (77 K) (i.e. for thickness on the order of the mean free path for inelastic and quasielastic scatterings and for a temperature with strongly reduced e-ph scatterings). At present we have no explanation for this pronounced discrepancy. We can only suspect that some dynamical details, in particular regarding the interface dynamics, are still missing in the present simulation scenario and become decisive in thick layers and at low temperatures. We should note that Bell (1996) has attempted to explain his experimental finding of a decreasing low-temperature BEEM current with increasing layer thickness by the decrease of multiple internal reflections and the corresponding decrease of the number of "attempts for transmission" at the interface. Our simulations confirm this dominance of multiple reflections in thin layers, but cannot reproduce the decrease of I_B with increasing d , because our theory lacks the $\underline{k}^{\parallel}$ -matching restrictions of Bell's forward injection scenario. Moreover, our reproduction of Bell's simulations revealed that his interpretation and the practically perfect agreement of his theoretical I_B/I_T versus V_T characteristics (dashed lines in Fig. 2) with the experimental data strongly depend on his choice of mean free paths and of the detailed injected current distribution: the calculated I_B changes drastically, (i) if the opening angle is e.g. changed from 10 to 20 degrees, or (ii) if the energetic window is changed from Bell's 0.2 to 0.4 eV, or (iii) if his mean-free path description is replaced by our detailed bulk-scattering dynamics in \underline{k} -space. So we believe that no convincing explanation exists for the decrease of I_B with increasing d at low temperature.

To summarize, the present \underline{k} -space description of the injection spectrum and of the bulk scattering dynamics has no adjustable parameter and therefore improves over the many-parameter fits of earlier theoretical interpretations. It turns out that scattering processes have no decisive influence on the spatial BEEM resolution. Although quantitative agreement with experiment is found in most cases, some remaining discrepancies seem to indicate the need for an improved description of the electron dynamics at the interface.

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current in metal

FIGURES
inelastic contribution

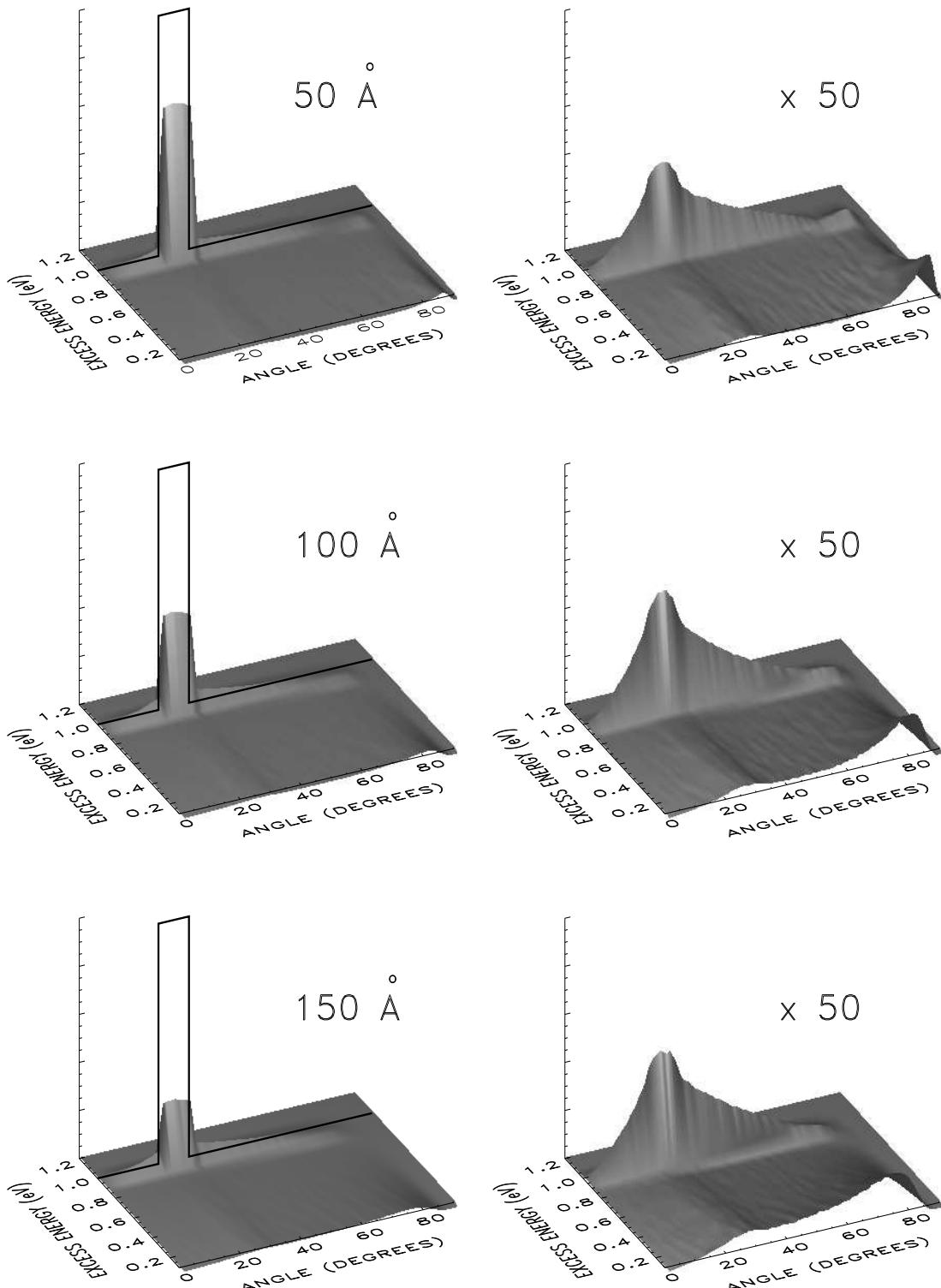


FIG. 1. Spatial evolution of current density in metal layer for injected distribution (at $z=0$) shown as solid line.

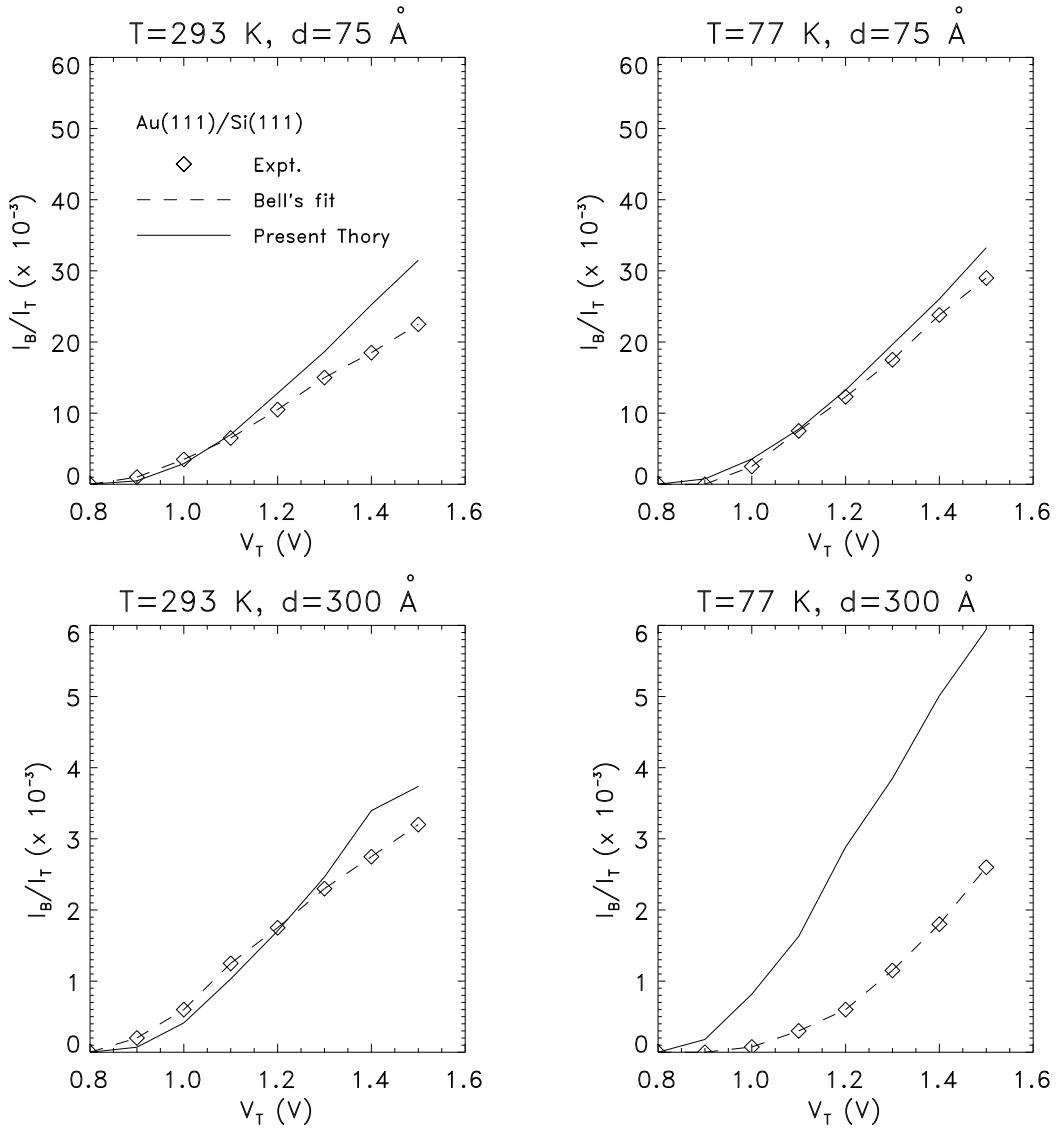


FIG. 2. Relative BEEM current versus bias voltage; experimental data taken from Bell 1996